efect A (helium, vacancy) from a
illed with n helium atoms

A (helium atom or vacancy) in a
lled with n helium atoms

m atom in a dislocation core filled

m atom in the core of a dislocation
atoms present in the core at some
om considered.

SUMMARY

The computer simualtion technique is applied to investigate the properties of point defects and line defects in metals. For that purpose crystallites are constructed in which these defects are simulated. In the case of line defects (dislocations) the initial positions of the atoms, surrounding the dislocations , are determined using the elastic theory of anisotropic media (chapter 2). Hereafter the atoms in such crystallites are allowed to relax to their minimum potential energy positions under the influence of the interatomic forces. These forces are derived from interatomic interaction potentials. These potentials are together with the boundary conditions of the simulated crystallite the main input data in these computer simulation models.

In chapter 3 extensive attention is paid to the interactions between the atoms in a crystal lattice. Main information on the interatomic forces and the derivatives of these forces can be obtained from the experimental phonon dispersion curves and elastic constants. The latter physical data, which have been used by various authors in potentials proposed, give a more limited insight than the former. In this chapter therefore, potentials are presented which have been fitted to the experimental phonon dispersion curves and the formation energy of a vacancy. Such potentials, however, are not unique. Additional information on certain interval of the potentials is necessary. In this chapter also a method is presented to include the migration
on certain intervals of the potentials is necessary. For that purpose in this chapter a method is presented to include the migration energy as an additional fitting constant. Using such potentials for bcc metals (Cr, Mo, Fe, W, Ta) and fcc metals (Pd, Ni, Cu, Ag, Au) some properties of point defects are calculated.

For molybdenum and copper the atomic configurations of edge and screw dislocations are investigated (chapter 4). The results, obtained in the computer simulation model (atomistic model), are compared with those obtained using the elastic theory of anisotropic media. Also the influence of the potentials used is studied. Special attention is paid to the dissociation of both the edge and screw dislocations into partial

dislocations. This phenomenon has been observed in our calculations for copper.

In chapter 5 the interaction between helium atoms and both point defects and dislocations is investigated. For that purpose, interaction potentials are derived describing the interaction between two helium atoms and potentials describing the interaction between a helium atom and a metal atom. These potentials are fitted to the activation energies of helium desorption from vacancies filled with helium atoms as experimentally measured in helium desorption experiments. Using these potentials the interaction of helium atoms with vacancies and with edge and screw dislocations in molybdenum is studied. For comparison the calculations have been repeated using potentials quoted in the literature. The results of the atomistic calculations are compared with the results obtained using the elastic theory.

SAMENVATTING

De computersimulatietechn
punt- en lijnfouten te onderz
simuleerd waarin deze fouten
fouten (dislocaties) worden d
deze dislocaties bepaald met
anisotrope media (hoofdstuk 2
worden vervolgens losgelaten
waarvoor hun potentiële energ
vinden plaats onder invloed v
leid uit interatomaire intera
samen met de randvoorwaarden
belangrijkste invoergegevens

In hoofdstuk 3 wordt uitv
wisselwerking van atomen in e
de interatomaire krachten en
afgeleid uit experimenteel ge
elasticiteitsconstanten. Laat
diverse auteurs in hun potenti
beperkter inzicht dan eerstge
ook potentialen voorgesteld,
krommen en aan de vormingsene
potentialen zijn echter niet
intervallen van de potentialer
om de potentialen aan te passe
zoals die experimenteel wordt
die voor zowel k.r.g metalen
(Ni, Pd, Cu, Ag, Au) zijn op
puntfouten (vacatures en inte

Voor de metalen molybdeen
rand- en schroefdislocaties or
computersimulatiemodel (atomi
resultaten verkregen met de el
Ook de invloed van de gebruikt